UCRL- 95478
PREPRINT

STATISTICAL MECHANICS OF HOT DENSE MATTER

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This paper was prepared for the
La Jolla Physics Symposium
University of California, San Diego
September 6-8, 1985

October 1986

Lawrence Livermore National Laboratory

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August 1986

ABSTRACT

Research on properties of hot dense matter produced with high intensity laser radiation is described in a brief informal review.

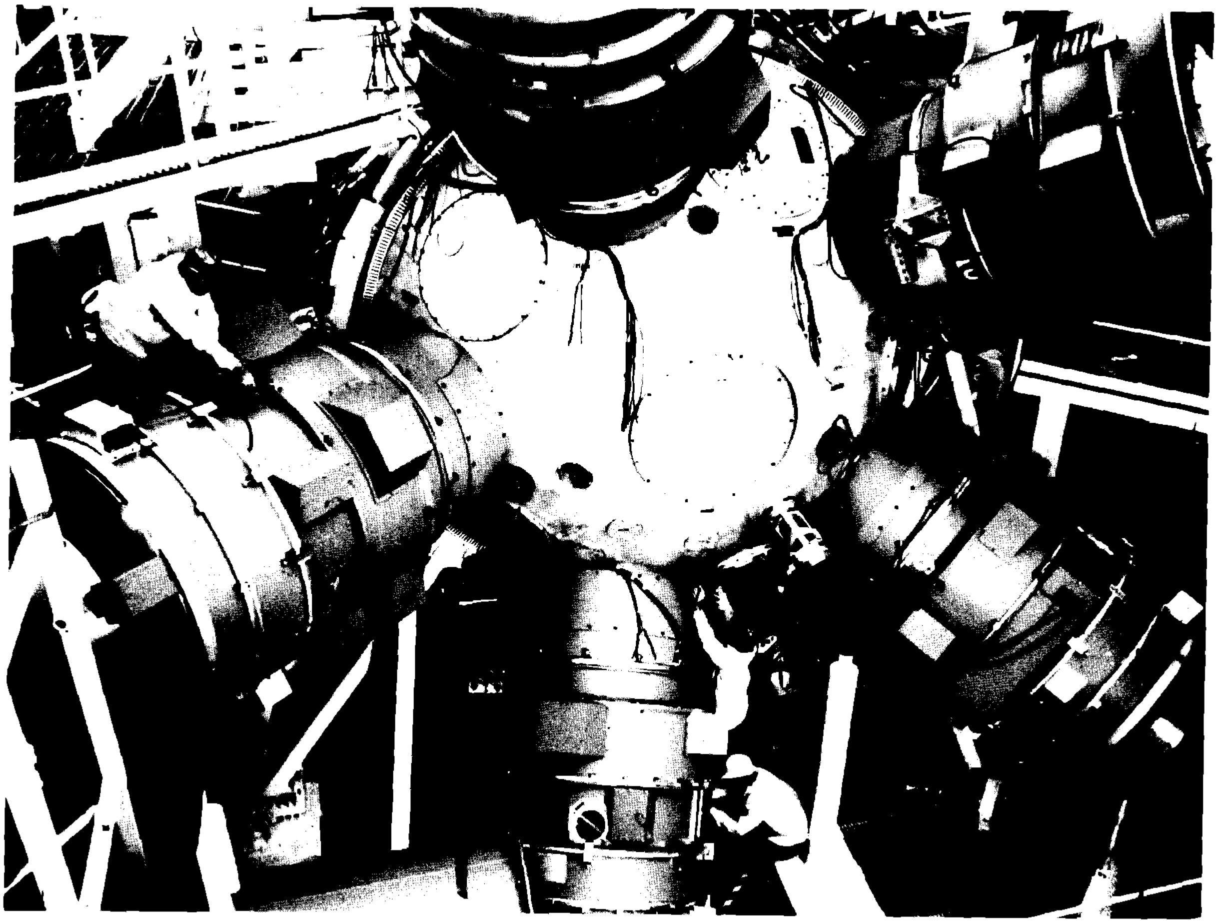

Fig. 1. Target chamber of the NOVA laser. Five large beam-lines are easily seen; these contain frequency-conversion crystals which convert infrared (1.06 μ) laser radiation to visible (.53 μ or .26 μ) light by nonlinear harmonic generation. The target, suspended in the center of the chamber can be as small as a pinhead and is heated to enormous temperature and pressure.

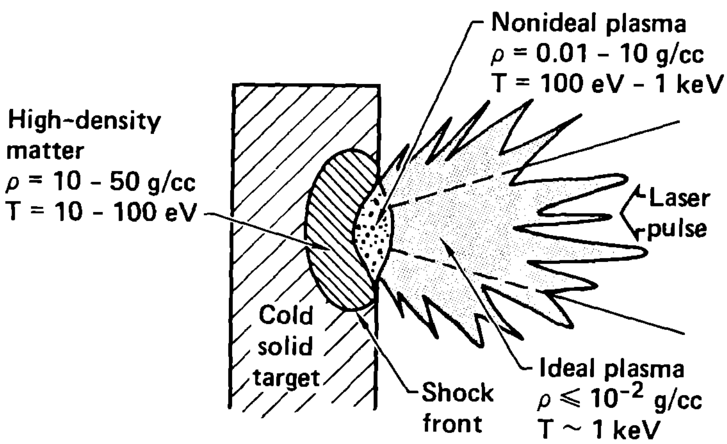

Fig. 2. Schematic laser-target interaction showing the different plasma conditions which are created.

LA JOLLA PHYSICS SYMPOSIUM UCSD

"Statistical Mechanics of Hot Dense Matter"

September 6-8, 1986

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(Introduced by Richard L. Morse)

At the beginning let me say that I could have been introducing Dick Morse and in that case the introduction would have been longer because his contributions to laser fusion are surely larger than my own. When the Los Alamos laser program started, Dick headed their theory effort. He wrote an early laser-target simulation code.[1] Dick and his group identified one of the main laser absorption mechanisms, called resonance absorption,[2] and they were the first to detect the anomalous heat conduction inhibition in laser plasmas as well as other phenomena in hydrodynamics and implosion symmetry.[3]

Many other La Jolla people participated in laser fusion. In ~ 1972 Keith Brueckner and his collaborators at KMS fusion published the first laser implosion experiments and Keith wrote two massive review articles summarizing those early efforts.[4] Chuck Cranfill, Yim Lee and I have also made some contributions.

Why work on laser fusion, large lasers and hot matter made with lasers? For myself there are several motivations, one is simply that these large lasers are beautiful things, and it is a pleasure to work around them. I've seen them evolve from table-top arrays of prisms and lenses to huge machines like accelerators; we keep hearing about new physics, new experiments, and novel ideas.

Another reason to work in this area is that our laboratory, which invests a lot of resources in building lasers, is determined to be the world leader in the technology, and so one is automatically pushed toward the front of the competition.

You can see another reason by looking at our latest laser, NOVA, and its target chamber (Fig. 1). If you compare it to the people, you see the scale is large. When a laboratory spends $200 million dollars on building a laser, then they believe they should spend a few dollars for theorists to tell them what targets to point it at. That means the theorists can think about physics and not worry about raising money.

Now these are reasons which got me into the subject, but actually things have changed in the last few years. It has become cheaper to build high-power lasers, and so we are seeing them pop up all over the world. There are productive laser research groups in France, England, Japan, Germany, Canada, and smaller efforts in Spain, Italy, Algeria, China, and the Soviet Union. It looks like we will soon have vigorous competition from University researchers who work on weekends and work late at night.

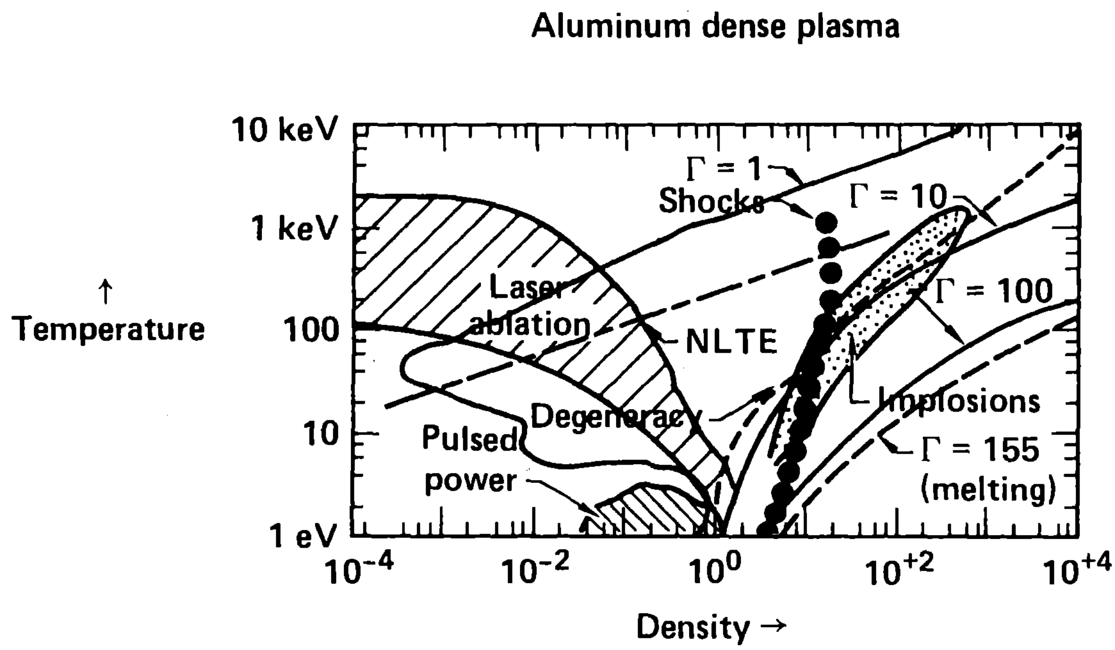


Fig. 3. An approximate phase diagram for matter at extreme high energy density, showing conditions reached in various plasma sources as well as some relevant theoretical parameter values.

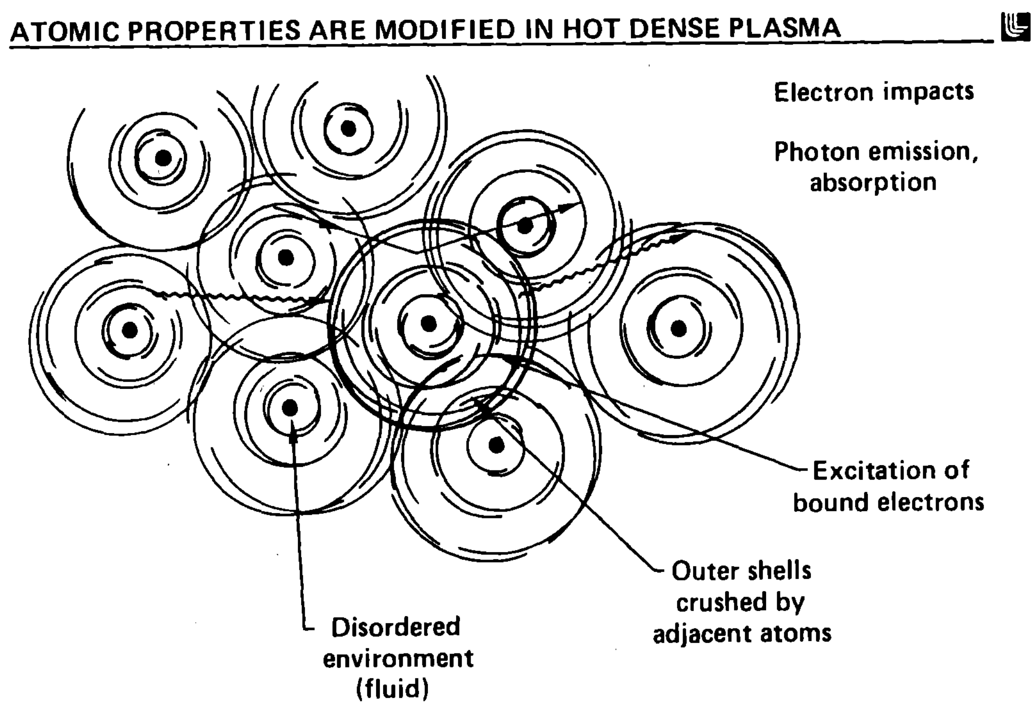
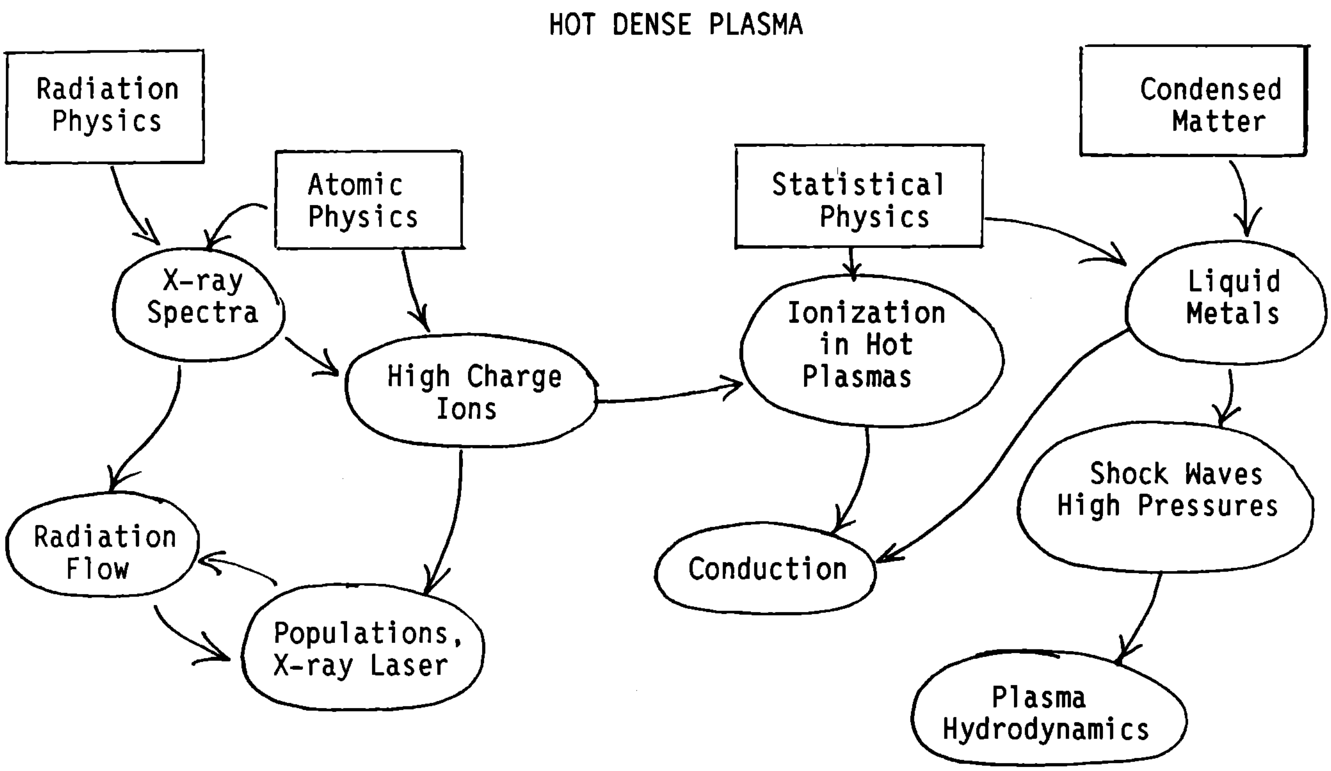


Fig. 4. Schematic overview of atomic phenomena in a high-density plasma. The circles surrounding the point nuclei are intended to represent the shells (1s, 2s-2p, etc.) of bound electrons. We have theoretical models that focus on the positions of atoms in the disordered environment and models that focus on the electrons of one compressed atom.

Apart from any practical application to generating energy, laser-heated targets generate some very interesting physics (Fig. 2). There is some material at high temperatures and low densities - material that is exploded out of the target and heated by the laser - this is the classical plasma. There is a dense plasma region gets very hot by laboratory standards and is very dense by plasma standards--densities like 10^{22} electrons/cm^3 or .1 g/cm^3, temperatures like 10^6 °K or 100 eV. Finally, there is a remarkable region of material compressed beyond ordinary solid densities to form high density matter in which atoms are pushed together and inner-shell electrons are perturbed. With lasers, we can make shock waves of 10-100 Mbars, and by conventional standards of high pressure physics that is very high pressure indeed.

I have a density-temperature phase diagram, and it shows some lines of the gamma parameter that Tom O'Neil mentioned (Fig. 3). This diagram shows you two things: first, there is a range of densities and temperatures in the targets. There is an ablation region; there is a compression region. And second, other plasma technologies also make dense plasmas. Of course, interiors of stars and large planets also reach conditions on this chart, so we have lots of interaction with other pure and applied science research.

Now, atoms in a hot dense plasma are squeezed, and their properties are modified, and that is the game (Fig. 4). Many atoms get pushed so close together that their outer edges touch; photons and free electrons scatter and perturb them. The game is to understand that complex situation.



Actually, the hot dense plasma is not only statistical mechanics, it involves every area of physics. We have a strong interest in the generation and propagation of radiation, especially x-rays. Also we combine ideas from atomic structure physics, statistical mechanics, and the physics of condensed matter. You can see connections to x-ray spectroscopy, radiation flow, calculation of the structure of highly charged ions, electron populations and x-ray laser action. Then again we study the ionization state and electron-ion scattering which enables us to calculate electrical conduction phenomena. To understand shock waves, we need to understand liquid metals, and that traces back to solid state physics.

I can only say a few words about each of these subjects. Let's start with the basic theoretical pictures. These are models which take the real situation and abstract out of it an idealized description that we can play with.

The first model is very heavily used; it is the model of point charges in a neutralizing background.[5] (See Fig. 4 again.) Of course, the point charges repel one another. One can follow them by the Monte Carlo method, invented by Marshall Rosenbluth among others,[6] which samples many pictures of the spatial location of the ions and decides which patterns are most likely. There is also the molecular dynamics method which treats the ions as point charges that move in time under Newton's law of motion with electrical forces and samples the time history of those motions for as much computer time as one can afford. These computer techniques help to answer the question, "Where are the ions?"

The gamma parameter that we just mentioned is

$$\Gamma = Z^2 e^2 / R_0 kT \tag{1}$$

where Z = ion charge, $R_0 = (3/4\pi n_i)^{1/3}$ = is the average distance between neighbor ions, T = temperature. Depending on the value of the Γ parameter you have very different physics ranging from ideal gas physics ($\Gamma \ll 1$) to crystalline state physics ($\Gamma > 178$). At typical laser-plasma conditions Γ is ~ 1 to 10 and the computer results show that the ions are repelled enough to make a sort of empty cavity of radius ~ R_0 around each ion.

The second model to describe a dense plasma is to focus on one atom (ion) and look at the physics of that atom by self-consistent field calculations. You would use this model if you were more interested in the electrons. The equations to solve are:

$$-\frac{\hbar^2}{2m} \nabla^2 \Psi_s + V(r)\, \Psi_s = \varepsilon_s\, \Psi_s \tag{2}$$

$$f_s = \frac{1}{1 + \exp(\varepsilon_s - \mu)/kT} \tag{3}$$

$$n(r) = \sum_s f_s \mid \Psi_s(r) \mid^2 \tag{4}$$

$$\nabla^2 V = - 4\pi(\rho_+(r) - en(r)) \tag{5}$$

There is a nucleus at the center of a cavity, and electrons around it and then you have an external environment which is a uniform positive and negative charge density that squeezes the atom. ($\rho_+(r)$ = constant for $r > R_0$; $\rho_+(r) = Ze\delta(\vec{r})$ for $r < R_0$).

You first guess V(r) and solve the Shrodinger equation, Eq. (2), for all the electron wave functions Ψ_s and energies ε_s. You assume the electron states are populated by Fermi statistics, Eq. (3), a basic law of statistical mechanics, and you add up the densities of those electrons in Eq. (4). Then you compute a new potential V(r) by solving Eq. (5). The problem is solved when the input potential in Eq. (2) agrees with the output potential from Eq. (5), and that's the calculation.

There are several things to debate in that calculation. One is whether you've got the plasma environment correct outside the atom ($r > R_0$). Obviously, you don't and so the question is what can you do about that? This question would take you back to the point charge models.

Instead of talking about that, one can ask about another assumption, the Fermi statistics, Eq. (3). Can that equation ever fail? [See Eqs. (9, 10) and Fig. 6 below.]

The most important quantity to calculate is the charge or ionization state of the atoms. Right now, I am thinking about the dense plasma where the ionization is strongly influenced by compression of the atoms; the outer bound electrons become free as a result of pressure. We want to describe that phenomenon with this self-consistent field model.

One of the things to examine is how bound electrons become free in terms of the self-consistent potential. Figure 5 shows a sample potential, V(r), and the same potential with the angular momentum barrier $\hbar^2 \ell(\ell + 1)/2\, mr^2$ added to it. You see there is a pocket in the total potential for $\ell = 2$. If the density is low enough, then that pocket is at negative energies and can hold a bound state, a 3d shell. If the density is higher the 3d shell becomes a <u>resonance</u> state. And if the density were still higher, the pocket would go away and one would have only free electron states for $\ell = 2$.

The resonance state corresponds to a quantized positive energy but that energy is not real, it is a complex energy $\tilde{E}_s = \varepsilon_s + i\Gamma_s$ because the electron in the resonance has a probability to tunnel out of the pocket and escape to infinity. The complex energy raises an interesting statistical mechanics question. How should you count resonance electrons? What is the Boltzmann distribution or Fermi distribution for resonance electrons? If you just plug a complex number into the usual formula you will get a complex probability. That doesn't sound right. Should you take the real part of the complex exponential or do you take the exponential of the real part of the energy or what?

$$\text{Prob} = \exp\left(-\,\text{Re}\left[\frac{\varepsilon_s + i\Gamma_s}{kT}\right]\right) \quad ? \tag{6}$$

$$\text{Prob} = \text{Re}\left[\exp\left(-\frac{\varepsilon_s + i\Gamma_s}{kT}\right)\right] \quad ? \tag{7}$$

$$\text{Prob} = \exp\left(-\frac{1}{kT}\sqrt{\varepsilon_s^2 + \Gamma_s^2}\right) \quad ? \tag{8}$$

Of course it doesn't make much difference if the width is very small, but what's the correct formula? We have done some study of that question and

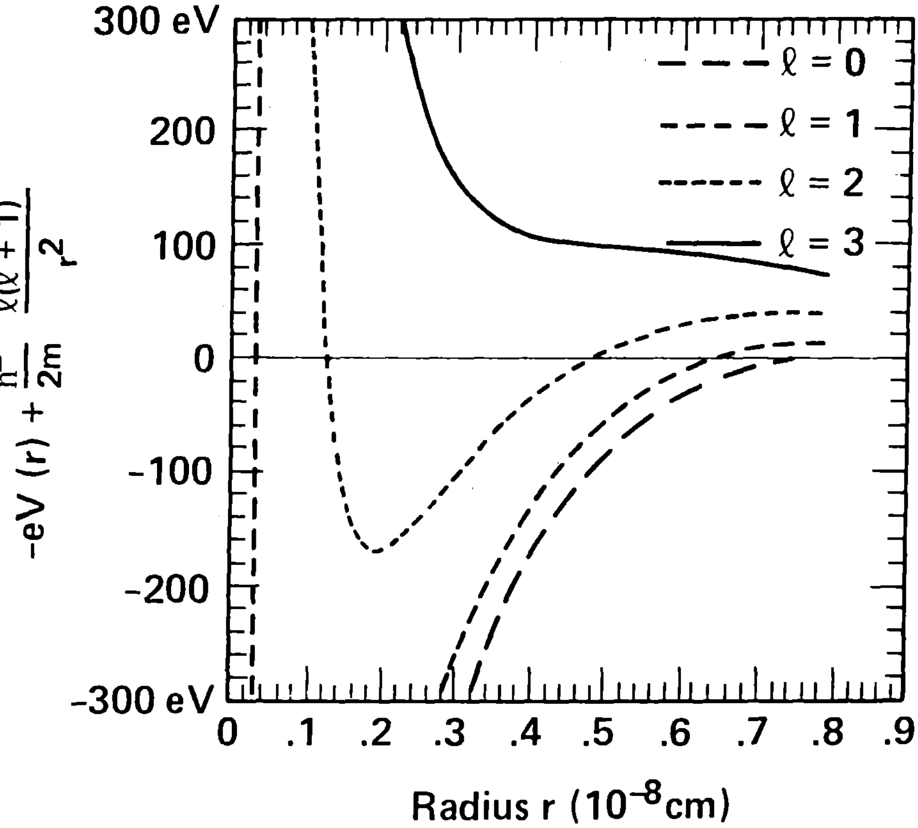


Fig. 5. Numerical self-consistent potential for Argon in a plasma of density 30 g/cm^3, temperature 1 keV. The $\ell = 2$ potential supports a low-energy continuum scattering resonance which has evolved through compression of the 3d shell of the isolated atom. The text quotes some statistical properties of such resonances in a finite-temperature electron system.

derived what we think is the exact answer.[7] This is a rigorous answer in a one-electron theory like the self-consistent field model and it generalizes Fermi statistics to states that have complex energies $\tilde{E}_s = e_s + i\Gamma_s$:

$$\text{Probability} = \text{Re}\,[F(\tilde{E}_s)] \tag{9}$$

$$F(\tilde{E}_s) = \frac{1}{i\pi} \int_0^\infty \left(\frac{\varepsilon}{\tilde{E}_s}\right)^{1/2} \frac{f(\varepsilon)}{\varepsilon - \tilde{E}_s}\, d\varepsilon \tag{10}$$

$$f(\varepsilon) = \text{Fermi function} = [1 + \exp(\varepsilon - \mu)kT]^{-1}$$

The equation says that the probability of finding the resonance state filled is the real part of a function $F(\tilde{E}_s)$ which is an integral over the Fermi function, containing the complex energy $\tilde{E}_s$ in two places. If the width is small, the real part of $\tilde{F}(E_s)$ reduces to the Fermi function $f(\varepsilon_s)$, but if the width is large, it doesn't. Now with an exact formula like this you ought to say precisely what the probability means, and here is an example: if you want to calculate the electron density $n(r)$, you must add up contributions of the following form, one term for each resonance state:

$$n(r) = \sum_s \text{Re}\,[F(\tilde{E}_s)\,\phi_s^2(r)] \tag{11}$$

The "resonance wave functions" $\phi_s(r)$ have their own precise definition.[8] These formulas are examples of some exact theorems for the self-consistent field model of resonance states.

There is another question of a statistical character about the use of Fermi statistics, Eq. (3), for the self-consistent field model. Fermi statistics are derived for non-interacting electrons. We have done some model calculations to examine the question whether Fermi statistics can be used for interacting atomic electrons.[9] I could try to explain the details, but it would take too long so I'll just show you an example. We find that Fermi statistics fails by about ten percent for an exactly soluble model system of many electrons, a model that is semi-realistic for complex atoms in hot dense plasmas. Figure 6 is a calculation for dense niobium plasmas with 200 volt temperature and gives the percent error in Fermi statistics for two of the shell populations. You see that Fermi statistics gets more accurate as you go to higher densities, and is poorer at lower densities. This behavior can be understood in terms of changes in the electron-electron interaction that is causing the effect.

Now, these are examples of statistical mechanics in the theory of dense plasmas. If I were giving this talk at Livermore, people would start to agitate in the audience and say, well, can you do anything useful? We've tried to do some useful things over the years. One is to look at the physics of energy loss of fast charged particles in hot partially ionized matter. Slowing down of fusion reaction-products is very important to thermonuclear burn. If you think about an ion or an electron moving through matter, the energy loss

$$\frac{dE}{dx} = -\frac{4\pi Z^2 e^4}{mv^2}\left\{n_I \log\left(\frac{2mv^2}{I}\right) + n_e \log\left(\frac{2mv^2}{\hbar\omega_p}\right)\right\} \tag{12}$$

appears to depend on the plasma temperature. There are several reasons, but the big effect is caused by ionization. When a charged particle moves past a neutral atom with bound electrons, the bound electrons cannot be excited or ionized unless they receive a certain minimum energy-transfer. The average energy transfer is the Bethe-Bloch mean excitation energy I. In Eq. (12), Z and v are the projectile ion charge and speed; n_e, n_I are target electron and ion densities and ω_p is the plasma frequency.

DETAILED CONFIGURATION CALCULATIONS RIGOROUSLY TEST AVERAGE-ATOM FERMI STATISTICS APPROXIMATION WITHIN THE HYDROGENIC MODEL

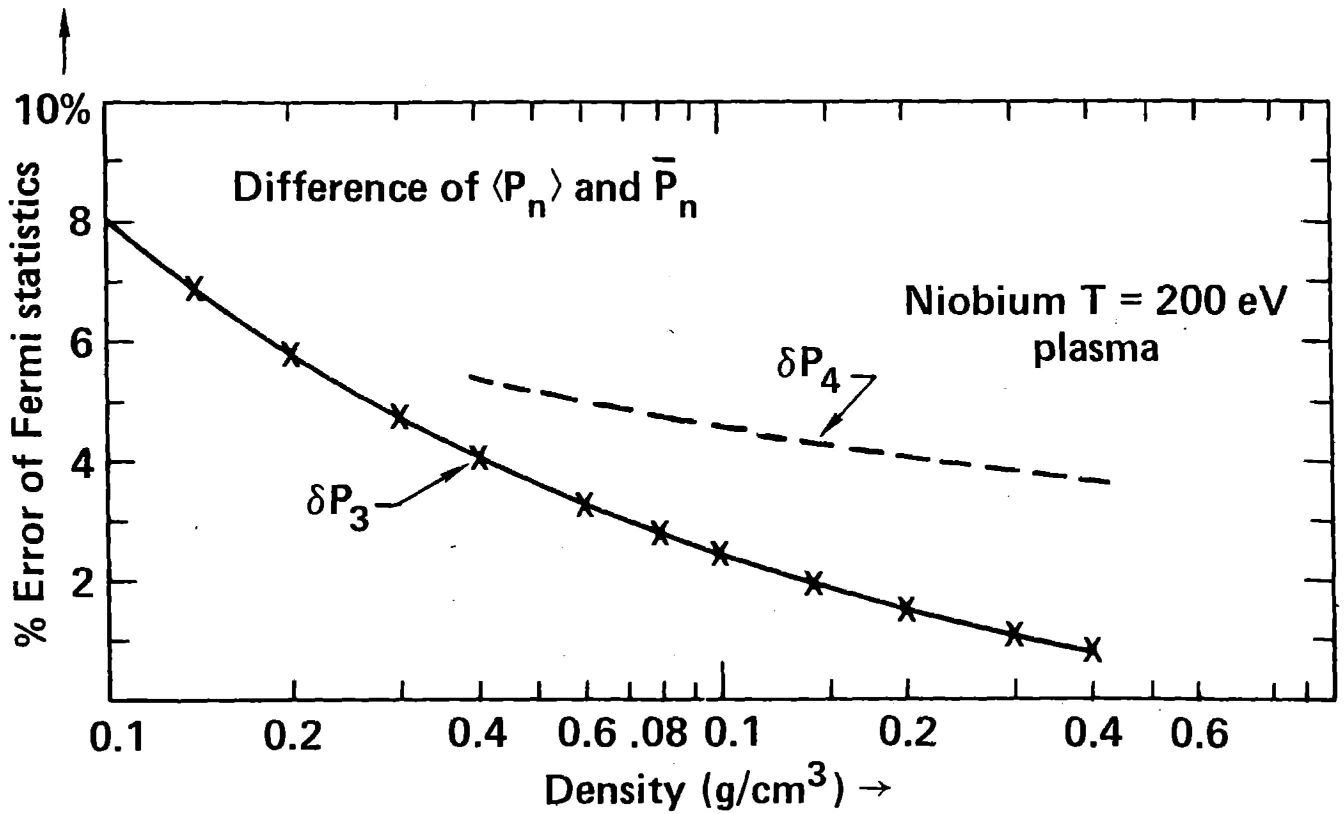


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Fig. 6. A numerical test of Fermi statistics for interacting electrons in atomic levels. < P_n > is the actual average population of the n^{th} shell (n = principal quantum number); P_n is the corresponding prediction of Fermi statistics.

When a target is heated, it gets ionized. It's outer electrons become free and then they can accept much smaller energy transfers ($\hbar\omega_p \ll I$), so they can accept energy even at a larger distances. Since there are many more electrons at the larger distances, this should raise the energy-loss. At Livermore, we calculated the quantity I, which is one of the key physical parameters in this parameters in this effect.[10] Our result for I is rather accurately reproduced by

$$I(Z,\ Q) = 10\ \text{eV} \cdot Z \cdot \frac{\exp\left[1.29\ (Q/Z)^{.72} - .18\ (Q/Z)\right]}{(1 - Q/Z)^{1/2}} \qquad (13)$$

where Z = nuclear charge, Q = ion charge.

Our calculation is done by a very simple method, Thomas-Fermi theory, but the results agree nicely with elaborate quantum mechanical calculations done by Gene McGuire of the Sandia Laboratories (Fig. 7). I don't have a picture of experiment versus theory, but there have been experiments to measure this. The experiments are not very precise, but they roughly agree with the theory.

Here is an example that shows how big is the predicted effect (Fig. 8). For a cesium projectile stopping in an aluminum target at three different temperatures you see that the predicted stopping power (the energy loss per path length) changes by more than a factor of two as you heat up the target to plasma temperatures. That's a big change and it affects the design of devices using fast ions to heat targets. The Thomas-Fermi formula for I is simple enough that we use it as a subroutine in our big laser-plasma code LASNEX.

OK, another subject, plasma hydrodynamics. One question of great interest is how much pressure can you make by shining your laser on a target? The answer will be sensitive to many pieces of the physics in the calculation. It is measured by looking at the speed of a shock wave as it crosses the target in one or two nanoseconds. One can measure that speed very

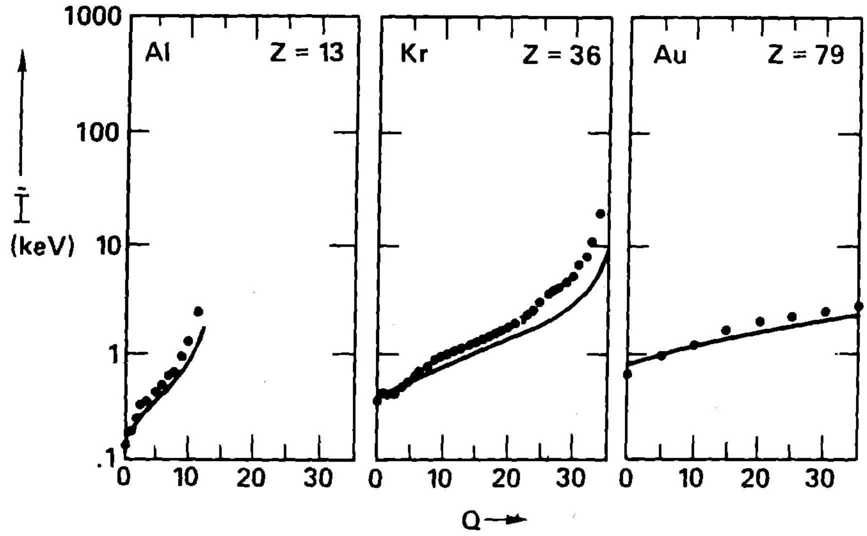

Fig. 7. Theoretical calculation of the average ionization-excitation potential I(Z,Q) for ions of Al, Kr and Au. Points are calculations by E. J. McGuire; solid curve is the Thomas-Fermi result of Eq. (13) and reference 10. The agreement is adequate for practical applications.

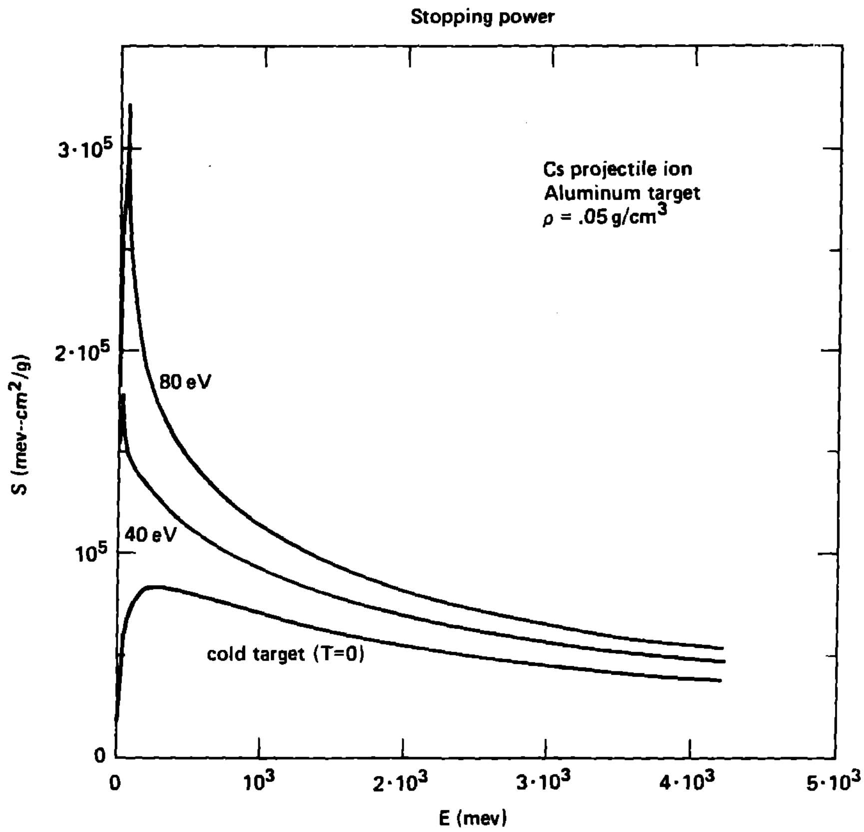

Fig. 8. Theoretical energy-loss (stopping power) of an aluminum target for Cs ion projectiles of various energies up to 5 GeV. The three curves are identified by the assumed target temperature. The temperature dependence shows the increased stopping effectiveness of free electrons produced by thermal ionization of the target plasma. The calculations are performed by a method described in Ref. 9.

accurately with fast streak cameras and then infer what was the plasma pressure at the point of laser impact. Here is a theoretical formula for the pressure which we worked out in 1979 using the LASNEX computer code:[11]

$$p = 8.6\ \mathrm{Mbar}\left(\frac{I_{TOT}}{10^{14}\ \frac{W}{cm^2}}\right)^{.82} \qquad (14)$$

I_{TOT} is the total laser intensity and about 30% of it is absorbed. Experimental data has been taken at a number of laboratories over the years, and it turns out that LASNEX is pretty close to the experiments (Fig. 9). Now, other people calculated p(I)--Ray Kidder calculated it, Claire Max calculated it using a theory that originally started with Dick Morse.[12] But those calculations got the power-law wrong; with LASNEX we got the right answer.

Large electric and magnetic fields are generated in laser targets, and so one is interested in the electrical properties of the plasmas. Now, of course, electrical properties of ideal plasmas are well known. Some people here in the room performed plasma conductivity calculations back in the fifties.[13] But we are thinking about dense partially ionized plasmas, and in that case the physics changes a bit. Over a period of years, we have done electrical conductivity calculations, stapling together ideas from plasma theory, atomic and solid state physics, and hopefully including enough physics to get the right answer.[14,15]

This is an example of the conductivity of aluminum (Fig. 10). The solid line is our result. It matches solid state data and theory down at low temperatures and at high temperatures it joins the ideal plasma theory, and in between, it predicts the electrical and thermal conductivity and their dependence on magnetic fields. I won't describe the calculation in detail,

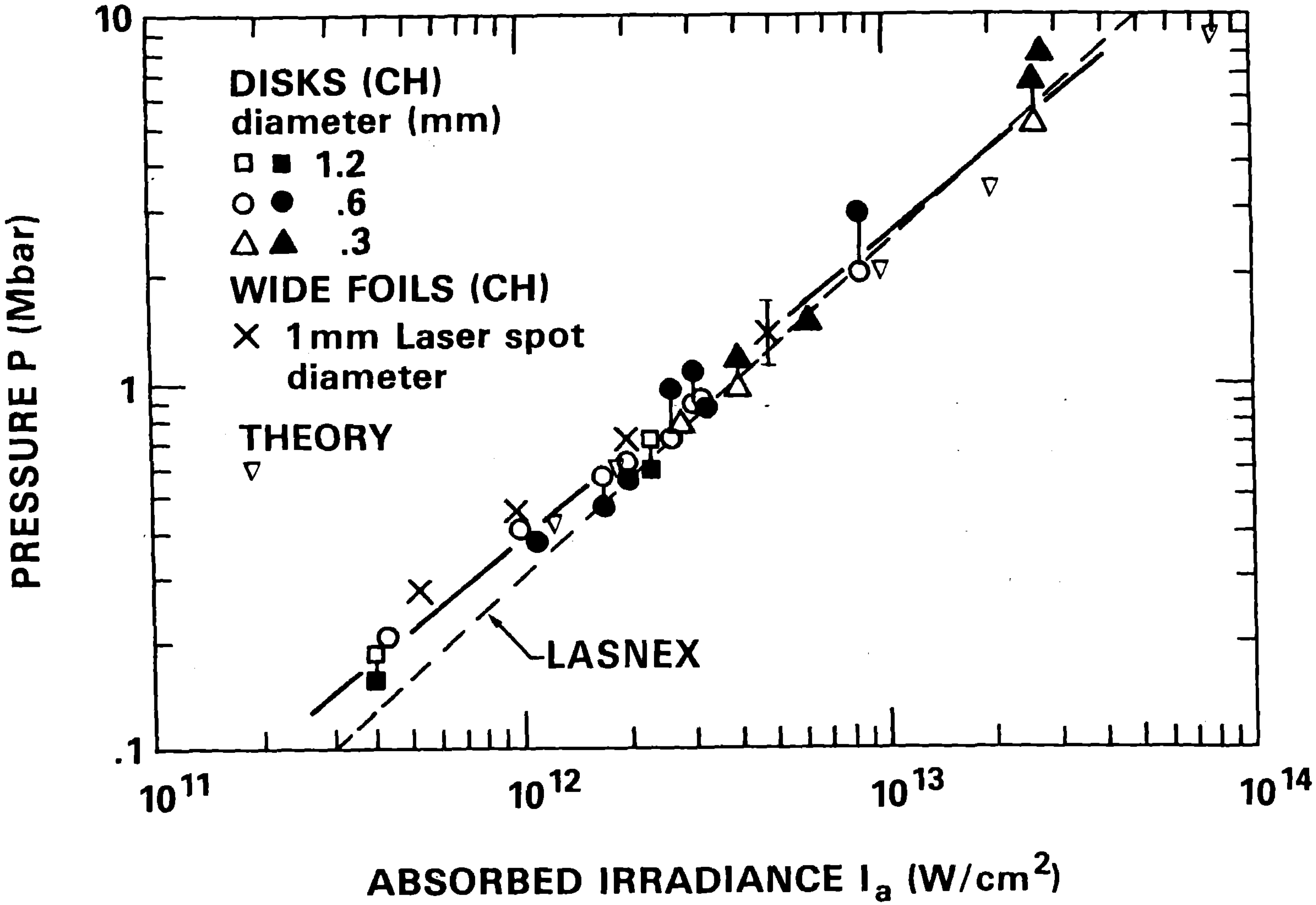

Fig. 9. Pressure generated in planar laser-target interaction at various laser intensities ($I_a \sim 1/3\ I_{tot}$). The experimental data is taken from U.S. Naval Research Lab Report 4212 (B. Ripin, et al.). The dashed calculation is Eq.(14), given first in Ref. 11.

but I can give you an idea of what the ingredients are: We have Maxwellian electrons or Fermi statistics depending on the density of the plasma. We have Coulomb scattering but also scattering by the ion core. There is provision for scattering by neutrals when they occur. We calculate the structure factor for dense plasma screening which converts over into Debye screening in the low density plasma. The electron mean free paths are sometimes as short as an atomic diameter. We use formulas that reduce to the Bloch-Grüneisen law for cold metals. However, we don't do a very good job on electron-electron scattering, and we don't include the process in which an electron hits an atom and excites or deexcites it and emerges with a different energy. We don't use the fanciest possible theory of screening, but you can't do everything. That is the TKN conductivity model, also part of LASNEX. It has been tested recently in experiments at Los Alamos and the University of British Columbia in Vancouver.[16] The code sees a lot of practical application in the study of exploding wires, fuses and so forth.

This conductivity model illustrates an interesting trend in large-scale computational physics, the need to build subroutine packages which represent a whole class of phenomena (e.g., conductivity) in a robust, broad-range fashion. Then the large code treats this package as a specialized expert on electrical properties.

Let's see. One more subject involving statistical mechanics: our laser plasmas are believed to be in a special kind of nonequilibrium state where the electrons have one temperature T_e and the ions have another temperature T_i. The temperatures are unequal because the large mass difference impedes heat transfer. For dense plasmas, one can develop a special new statistical mechanics, a canonical ensemble based on the idea that particles (electrons, ions) interact strongly with each other but the temperatures are unequal.[17]

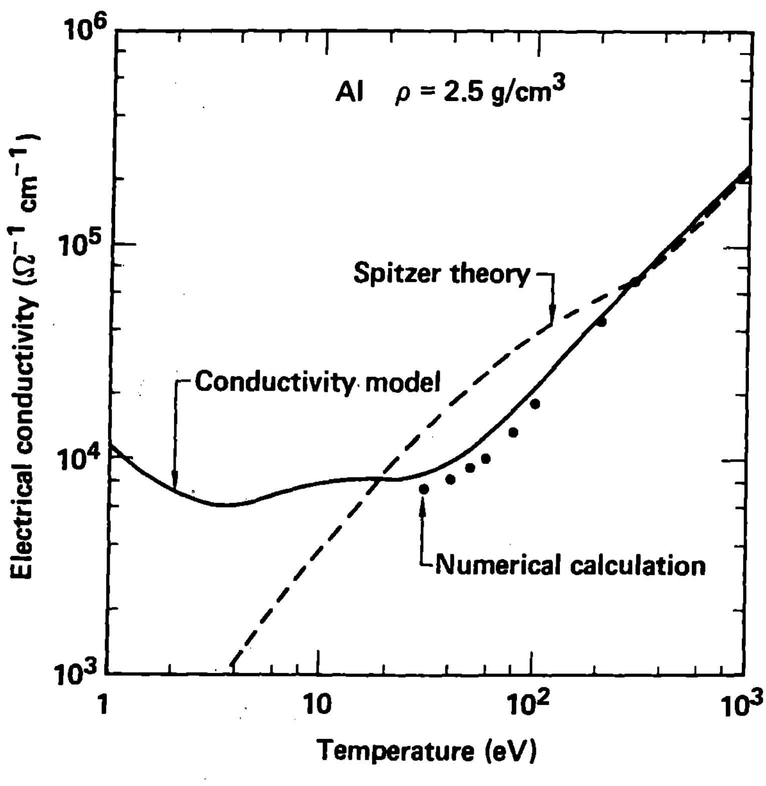

Fig. 10. Theoretical electrical conductivity for hot dense aluminum calculated by the model of Lee and More (ref 15). At low temperatures this approaches the correct metallic result, which is very different from the Spitzer plasma theory. The region near 10 eV corresponds to strong electron-ion scattering with a mean free path as short as the atomic diameter. The calculations are partially verified by experiments reported in Ref. 16.

Then the thermodynamic relations become a bit more complicated and interesting. For example, we find a modified formulation of the first/second laws of thermodynamics:

$$dE = T_e dS_e + T_i dS_i - pdV \tag{15}$$

We find that the specific heat becomes a sort of matrix--If you add heat to the electrons, then you automatically change both temperatures (T_e and T_i) because you change the ionization state and the ion pair-forces. All this gives a very pretty theory, which has not yet had any real experimental test.

We want to know the ion temperature because it controls the rate of thermonuclear reactions in fusion plasmas, and and it also determines the Doppler line width, which controls the gain of x-ray lasers.

I'll barely have time to mention the last subject. Of all the things that I've worked on, this turned out to be the most important. It's not my fault that it did; it wasn't even my idea to work on this. The original idea came from Russell Kulsrud, Marvin Goldhaber, and others; the idea is to use <u>spin polarized fuel</u> in fusion reactors.[18] The Princeton group worked out this idea for magnetic fusion, and at Livermore John Nuckolls suggested we should think about it for laser fusion. It turned out to be a wonderful idea. The big consequence of having spin polarized DT (deuterium-tritium) nuclei is to increase the thermonuclear fusion reaction cross section by about fifty percent. Let's try to imagine fusion targets with spin polarized DT nuclei undergoing fusion reactions. We must ask several questions. Can you polarize DT nuclei in the first place? Can you polarize them in an actual target capsule that you could put in front of a real laser? Would the polarization still exist after you imploded the target? (My calculations seem to say "yes" to this one.[19]) And finally, would you get a significant

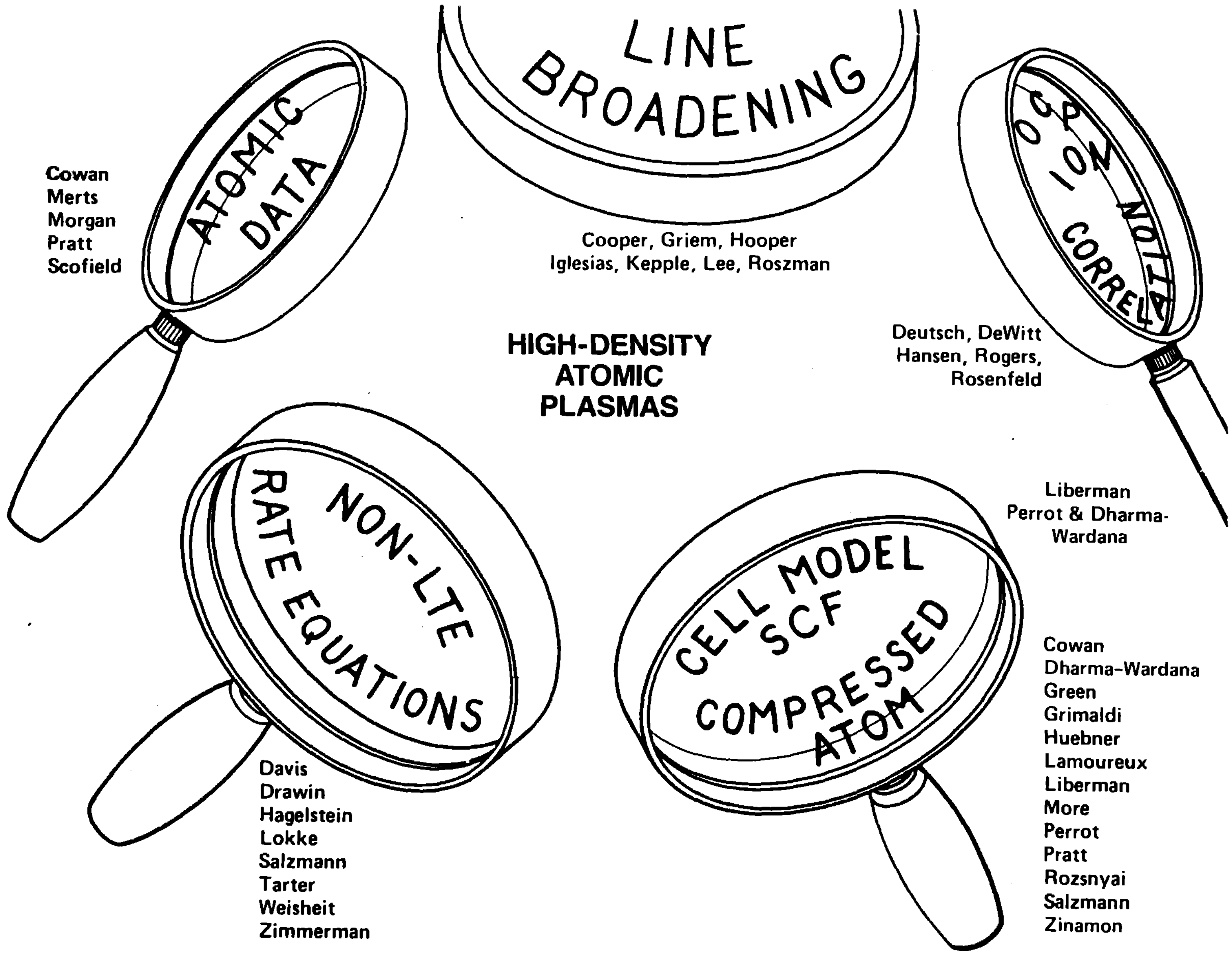

Fig. 11 The high-density atomic plasma can be viewed from several viewpoints in which one important aspect is brought into clear focus. The names given are merely a sampling of the many active scientists in the field.

improvement in target performance? I will just say a word about that last question. Recent LASNEX theoretical calculations show that a target with polarized fuel would perform very much better than a target with unpolarized fuel, and you could cut the laser size by a factor of two or three.[20] Since the laser costs two hundred million dollars, or five hundred million dollars or a billion dollars, you are talking about a very significant financial savings by going to spin polarized thermonuclear fuel. We are trying to encourage solid state physicists to develop techniques for spin-polarizing DT cryogenic solid fuel. We have a project underway at Livermore to do that.

Let me end with an over-view of the high density plasma seen from different points of view. When people with these different points of view see a plasma, they may see different things (Fig. 11). For example, the x-ray laser people see dense plamas as being a place to exercise rate equations and move atomic populations. And, if you look at the fine print you will see that nowadays there are many researchers working on these subjects.[21]

Acknowledgements

Work performed under the auspices of the U.S. Department of Energy by the Lawrence Livermore National Laboratory under contract number W-7405-ENG-48.

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21. Figure 10 does not attempt to list all the many researchers in the dense plasma field, and is several years old in any case. One can get a reasonable overview of the field from the recent conferences on dense plasmas; see, J.Q.S.R.T. Vol. 27 (1982), or proceedings (to appear) of international conferences in Williamsburg, Va. (1985), Cargese, Corsica (1985) and St. Andrews, Scotland (1985).